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Limitations and potentialities of computerised glow curve deconvolution (CGCD) in the kinetics formalism

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Abstract : The limitations and potentialities of computerised glow curve deconvolution (CGCD) is illustrated taking into consideration a set of glow curves of an orthoclase feldspar ($KAlSi_3O_8$). It has been shown that CGCD can be a useful technique to extract meaningful trapping parameters provided one follows a logical method in data handling

Keywords : Thermoluminescence (TL), activation energy, orthoclase feldspar ($KAlSi_3O_8$)

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1. Introduction

Computerised glow curve deconvolution (CGCD) is on the verge of creating a mini revolution in the various fields of thermoluminescence (TL) research [1-3]. As on today, most of the CGCD works have been performed in the framework of the kinetics formalism which is based on three trapping parameters namely the activation energy (E), the frequency factor (s) and the order of kinetics (b). Though the order of kinetics (b) has no physical meaning for values other than $b = 1$, 1.5 and 2, the formalism is a useful concept basically for two reasons. Firstly, it gives a mathematical description of the phenomenon and many experimental glow curves can be described with reasonable degree of confidence following this model. Secondly one can estimate the lower limit of lifetime of the electron (τ) using the relation $\tau = 1/s \exp(E/kT)$ which is required for checking the suitability of a particular peak for dating [4]. Therefore. CGCD is potentially a powerful technique since amongst all methods of analysis it may be thought of as the most rigorous one. However, CGCD has failed to provide the much needed evidence of uniquely extracting the intrinsic trapping parameters (E and s), justifying thermoluminescence (TL) as a spectroscopic technique [5].

This paper is aimed in demonstrating that CGCD can be a useful technique in extracting meaningful trapping parameters provided a logical method is followed in handling the data. A set of glow curves of an orthoclase feldspar obtained after various thermal cleaning have been taken as an illustrative example to demonstrate the limitations and potentialities of CGCD.

2. Experimental

All the TL curves are recorded using the commercial recording system model TL 1404 (Indotherm Instruments Pvt. Ltd., Mumbai). The 15 min X-irradiated (30 kV, CuK_α radiation) thin samples ($5 \times 5 \times 0.05$ mm) of an orthoclase feldspar (Indian origin) are subjected to various amount of thermal cleaning (210, 220, 230, 240 and 250°C), and their glow curves are recorded with a uniform heating rate of 0.833°C/sec. The glow curves are recorded on a two pen strip chart recorder.

3. Results and discussion

TL curves of 15 min X-irradiated orthoclase feldspar subjected to various extent of thermal cleaning are presented in Figure 1. In all the cases, a single broad peak is observed.

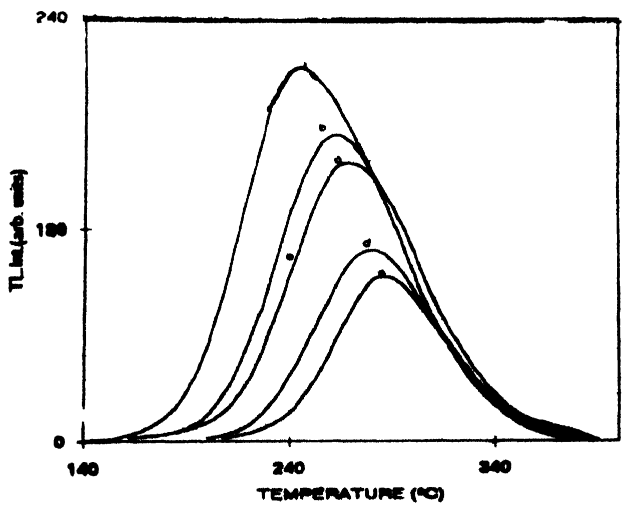


Figure 1. TL glow curves of 4 min X-irradiated orthoclase feldspar followed by thermal cleaning upto (a) 210°C, (b) 220°C, (c) 230°C, (d) 240°C and (e) 250°C respectively.

The characteristic peak parameters of the peaks are presented in Table 1. The shape factors $\mu_g = (T_2 - T_m)/(T_2 - T_1)$, (when T_m is the peak temperature while T_1 and T_2 are temperatures at half of the maximum intensity on the rising and falling sides of the peak) are in the range of 0.54 to 0.59, indicating that the peaks follow general order kinetics.

Broad glow peaks are not uncommon in feldspar in the sense that feldspar dominant meteorites are well knwon to exhibit such peaks [6–8]. TL of meteorites have been actively

Table 1. Peak parameters of thermally cleaned glow peaks of orthoclase feldspar

Thermal cleaning temp. T_C (°C)	Peak temp T_m (°C)	$\tau = T_2 - T_m$ (°C)	$\delta = T_2 - T_1$ (°C)	$\omega = T_2 - T_m/T_2 - T_1$ (°C)	Shape factor μ_g
210	246	34	50 0	84.0	0.59
220	262	33	45 0	78.0	0.58
230	268	33	42 4	75.4	0.56
240	280	33	38 4	71.4	0 54
250	285	29	35 0	64.0	0.55

studied and it has enabled new insights into low-grade metamorphism and evitrification, shock, brecciation and the postulated Martian origin of certain meteorites [9]. Therefore, CGCD of such curves have immense practical utility. Since each of the glow curve (Figure 1) seems to consist of a single peak we have performed CGCD using the program given in the book of Chen and Kirsh [10]. However, while handling the data in one case we have tried to fit the rising side (up to T_m) and in the second case we have used the whole

Table 2. Trapping parameters obtained by CGCD with single peak

Specification (°C)	Rising side curve fitting			Whole curve fitting		
	E (eV)	b	s (sec^{-1})	E (eV)	b	s (sec^{-1})
$T_c = 210$	1.35	4.0	5.9×10^{11}	1.16	2.28	6.5×10^{9}
$T_c = 220$	1.40	4.0	$5\ 8 \times 10^{11}$	1 23	2 59	1.5×10^{10}
$T_c = 230$	1 33	2 5	$1\ 1 \times 10^{12}$	1.27	2 50	$2\ 6 \times 10^{10}$
$T_c = 240$	1 54	4 0	$4\ 6 \times 10^{12}$	1 36	2.28	$9\ 7 \times 10^{10}$
$T_c = 250$	1.55	1.6	$4\ 8 \times 10^{12}$	1 63	2 55	$2\ 7 \times 10^{13}$

glow curve as one peak. The results of CGCD are presented (in Table 2). Some of the fittings are shown in Figures 2 and 3.

In all the cases, the rising side of the glow peaks fit well to the numerically computed ones. However, the falling side shows total disagreement. This is not surprising since such fitting predicts kinetics parameter (b) as large as 4, totally unknown in the literature of TL (Table 2). Hence, this set of trapping parameters have no physical significance (the consequence will be discussed later). The whole curve-fitting results show that there is mismatch in the entire region of the curve (Figure 3). Based on this we conclude that the simple looking broad curves cannot be fitted to single peaks. Rather they seem to consist of more than one elementary peaks.

There is no clear-cut procedure to deconvolute the peaks and find out the components. After certain amount of trial and error, we have succeeded in deconvoluting

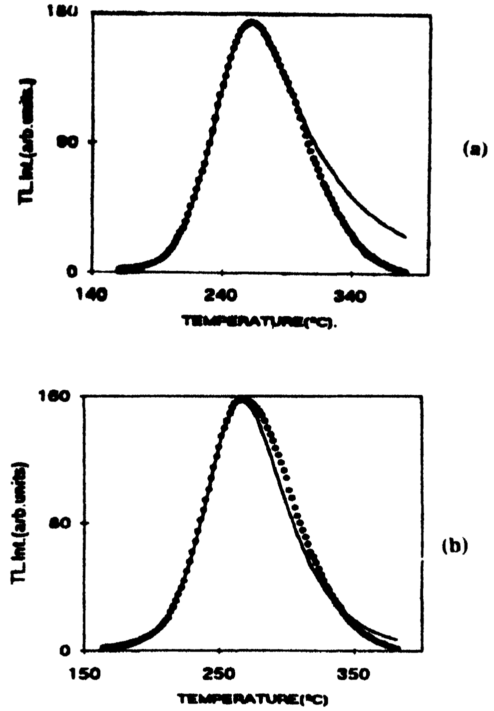


Figure 2. Rising side curve fitting of TL of 4 min. X-irradiated orthoclase feldspar followed by thermal cleaning upto (a) 220°C and (b) 230°C respectively.

●● Expt. curve ——— Theoretical curve.

Fitted parameters : (a) $E = 1.40$ eV, $b = 4.0$, $s = 5.8 \times 10^{11}$ sec^{-1} and (b) $E = 1.33$ eV, $b = 2.5$, $s = 1.1 \times 10^{12}$ sec^{-1}.

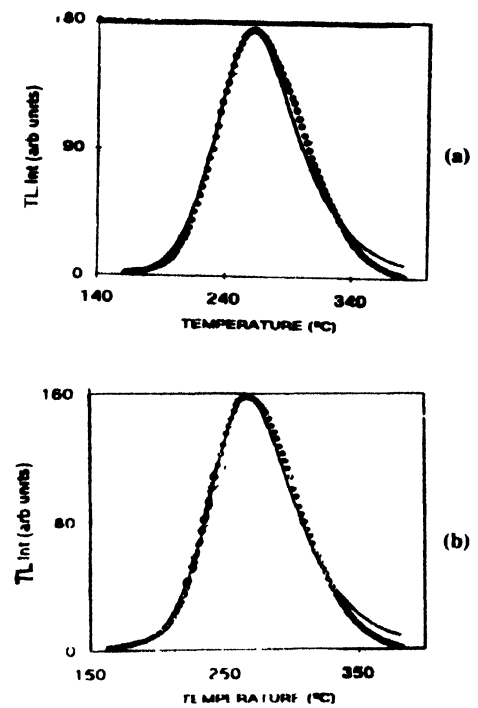


Figure 3. Whole curve fitting of TL of 4 min. X-irradiated orthoclase feldspar followed by thermal cleaning upto (a) 220°C and (b) 230°C respectively.

●● Expt. curve ——— Theoretical curve.

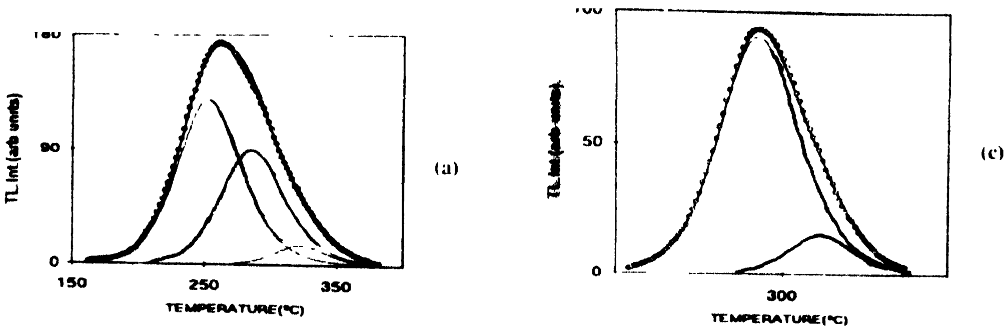
Fitted parameters : (a) $E = 1.23$ eV, $b = 2.59$, $s = 1.5 \times 10^{10}$ sec^{-1} and (b) $E = 1\ 27$ eV, $b = 2.50$, $s = 2.6 \times 10^{10}$ sec^{-1}.

the peaks. Some of the results are shown in Figure 4. The fitting in all the cases is good. The values of the trapping parameters are presented in Table 3. All the glow peaks

Table 3. Results of CGCD with multiple peaks.

Specification (°C)	Peak temp. T_m (°C)	E (eV)	s (sec^{-1})	b
	252	1.42	1.0×10^{11}	2
$T_c = 220$	285	1.59	1.0×10^{13}	2
	322	2.20	6.6×10^{18}	2
	256	1.44	2.3×10^{12}	2
$T_c = 230$	285	1.59	1.0×10^{13}	2
	322	2.20	6.6×10^{18}	2
$T_c = 250$	285	1.59	1.0×10^{13}	2
	322	2.20	6.6×10^{18}	2

are found to follow second order kinetics. This is in agreement with the analysis of glow curves of a number of feldspars performed in our laboratory [11–14]. Incidentally, the fact



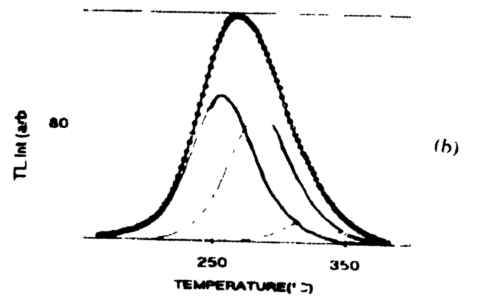


Figure 4. Deconvolution of TL of 4 min. X-irradiated orthoclase feldspar followed by thermal cleaning upto (a) 220°C, (b) 230°C and (c) 250°C respectively.
●● Expt. curve - - - Deconvoluted curve ——— Sum of the deconvoluted curve

that glow curves of feldspar follow non-first order kinetics, has been accepted in TL literature [3].

4. Limitations and potentialities of CGCD

Coming to the real motivation of the work, now we can comment on the limitations and potentialities of CGCD. In the present study, the rising side (upto T_m) of all the glow curves could be fitted with the three parameter (E, s and b)-kinetics formalism. Though the values of E and s are realistic, the b values are not only random but abnormally high (as large as 4). Thus, one can conclude that even when the fitting is deceptively precise, CGCD may not yield meaningful data. The misfit of the whole glow curve to numerical ones reveals the complexity of the simple looking glow curves. Here lies the potentiality of CGCD as a technique to decode the glow curve.

The glow curves could be fitted with a combination of two or three glow peaks. However, even in this case, the values of E and s for the 322°C peak is abnormally large, something similar to the case of the dosimetry peak of TLD-100 [2]. Thus the problem of decoding the glow curves is only partially solved.

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References

[1] A J J Bos, T M Piter, J M Gomez Ros and A Delgado *GLOCANIN, IRI-CIEMAT Report* 131-93-005 IRD-Delft (1993)

[2] Y S Horowitz and D Yossian *Radiation Prot. Dosim.* **60** 1 (1995)

[3] S W S Mckeever, M Moscovitch and P D Townsend *Thermoluminescence Dosimetry Materials : Properties and its Uses* (Nuclear Tech. Pub. Ashford Kent, England) (1995)

[4] M J Aitken *Thermoluminescence Dating* (London : Academic) (1985)

[5] R K Gartia *Luminescence and its Applications 97 (Proceedings of the NCLA-97* Oct 13–15) (Delhi : Allied Publishers) 59 (1997)

[6] R K Guimon, P K Bradly, S Weeks, J D Hart and S W G Sears *Geochimica et Cocchimica Acta* **49** 1515 (1985)

[7] F A Hasan, M Hag and D W G Sears *Geochimica et Cocchimica Acta* **50** 1031 (1986)

[8] B D Keek, R K Guimon and D W G Sears *Earth Planet. Sci. Lett.* **77** 419 (1986)

[9] D W G Sears, J M Dettart, F A Hassan and G E Lofgren *Chapter 11* in *Spectroscopic Characterization of Minerals and their Surfaces* eds L M Coyne, S W C McKeever and D F Blake (ACS Syposium Series 415) (1989)

[10] R Chen and Y Kirsh *Analysis of Thermally Stimulated Process* (Oxford : Pergamon) (1981)

[11] A B Ahmed and R K Gartia *Phys. Stat. Sol. (a)* **44** 645 (1985)

[12] A B Ahmed and R K Gartia *Phys. Stat. Sol. (a)* **98** K63 (1986)

[13] R K Gartia, S J Singh and A B Ahmed *Phys. Stat Sol (a)* **103** 593 (1987)

[14] A B Ahmed, R K Gartia and P S Mazumdar *J. Mater. Sci.* **23** 3683 (1988)